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Atomistic simulations for ceramic-metal interfaces: {222}MgO/Cu

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Ab initio local-density-functional-theory (LDFT) total energy calculations within the plane-wave pseudopotential representation are performed on {222}MgO/Cu in order to (i) design a model interface potential for use in large-scale atomistic simulations that include interface misfit, by Seidman and coworkers. Our LDFT calculations show that the (polar) {222} interfaces (either termination) have higher works of adhesion W than (neutral) {100} interfaces; experimentally, only the {222} orientation has been observed at precipitate interfaces in internally oxidized Cu(Mg) specimens. Most of the detailed calculations are for the O-terminated {222} interface, the one both observed experimentally, and predicted to have the largest work of adhesion. Electronic properties (densities of states, electron density distributions) for this interface are discussed. We present a model interface potential that includes two contributions: an interface-separation dependent (one-body) potential in the form of the "universal-binding energy curve", and a repulsive Born-Mayer-like two-body term. Molecular dynamics simulations are performed of the interface structure based on this potential.

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